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Optimization Of ISOL Targets Based On Monte-Carlo Simulations Of Ion Release Curves *

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Abstract

A detailed model for simulating release curves from ISOL targets has been developed. The full 3D geometry is implemented using Geant-4. Produced particles are followed individually from production to release. The delay time is computed event by event. All processes involved : diffusion, effusion and decay are included to obtain the overall release curve. By fitting to the experimental data, important parameters of the release process (diffusion coefficient, sticking time, ...) are extracted. They can be used to improve the efficiency of existing targets and design new ones more suitable to produce beams of rare isotopes.

Key words : ISOL targets; Release curve; Diffusion; Effusion; Monte-Carlo simulation; Geant-4.

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1 Introduction

Studying nuclear structure at the limits of the chart of nuclides, especially near the proton and neutron drip-lines, requires high intensity radioactive beams not available at existing facilities. Since the most exotic nuclei have the shortest half-lives, the time from production to extraction (release) from the ion-source, called "delay time", has to be the shortest possible. The release process involves the transport of produced nuclei first through the target material (diffusion) then through the target container and ionizer (effusion). The aim of this work is first, to identify the dominant process in the release of a given isotope and second, to reduce the delay time in order to increase the efficiency of ISOL targets to produce intense beams of rare isotopes.

The delay time is a function of the radionuclide species, target material, geometry, and the experimental conditions. In this work, we are interested in optimizing the target geometry for a faster release. This concerns mainly, the thickness, shape and arrangements of the target material inside the target container. For this purpose, we have developed a Monte-Carlo Model where the geometry is implemented using Geant-4 to which the effusion process has been added. The diffusion process is treated analytically using the corresponding solution of Fick's equation. The decay is applied afterward to the generated delay time distribution to obtain the final release curve.

A description of the calculation is given in the next section. In section 3, the calculation is applied to the case of the RIST target which has been tested at ISOLDE-CERN. In section 4, we study two effects that could directly affect the release process and explain the difference between measured and simulated release curves, namely the non uniform temperature in the target and the electric field in the ion source. Possible ideas to optimize the geometry and improve the efficiency of the RIST target will be discussed in section 5. Conclusions and future plans will be presented in section 6.

2 Description of the Calculation

Since the shape and dimensions of the target could help in making the release faster, it is very important to be able to choose the target geometry in order to minimize the delay time. Using the power of the tool kit Geant-4 [1], it is possible to implement any complicated 3D-geometry and modify it easily. The diffusion and effusion processes are treated separately, diffusion analytically and effusion in Monte Carlo.

The diffusion is treated using an analytical formula which is the solution of Fick's equation [2] for the corresponding target type (thin films, fibers or grains). In this paper, only targets composed of multiple layers of thin refractory foils are considered. For thin foils, the formula is :

$$P_d(t) = \frac{8}{\pi^2 \tau_d} \sum_{n=0}^{\infty} \exp(-(2n+1)^2 \frac{t}{\tau_d})\ ; \ \ \tau_d = \frac{d^2}{\pi^2 D}$$

This formula gives the probability for a particle to diffuse out of the target foil at a time t. The diffusion is characterized by the time τ_d at which about 70% of particles have left the target material. d is the thickness of the foil and D is the diffusion coefficient, a function of particle/target properties and the temperature. The formula is randomized to generate the diffusion time, t_d, event by event.

For the effusion, a special routine has been written and added to the list of physics processes of Geant-4. This new process considers the thermal motion (Maxwell motion) of a particle inside the target volume and treats its collisions with the encountered surfaces. At each collision, the particle sticks to the surface (adsorption, Frenkel's equation [3]) then it is re-emitted (desorption) to the target volume in a direction obeying the cosine distribution (Knudsen Law [4, 5]). The calculation is stopped when the particle leaves the ionizer. For each event, the total path length and the number of collisions with the surface are computed. They are used respectively to determine the flight time and the total sticking time. For the flight time, the mean velocity of the corresponding Maxwell distribution is used. The effusion time, t_e, is the sum of the flight and sticking times.

The total delay time is then obtained by adding the diffusion and effusion times: $t_d + t_e$. At this stage, we have the delay time distribution before decay. To consider the decay of nuclei while diffusing and effusing through the target and obtain the final release curve, the decay factor: $\exp(-\lambda t)$ is applied to the distribution of delay times. This curve can then be integrated to determine the efficiency for release of the isotope with a given lifetime. Other isotopes of a given element, but different lifetimes can be evaluated without repeating the time-consuming part of the calculation.

3 RIST Target Simulation

The Radioactive Ion Source Test (RIST) target [6] was designed and constructed at Rutherford Appleton Laboratory, UK and tested at ISOLDE-CERN [7]. The target container is a 20 cm-long, 2 cm diameter tantalum tube. It is filled with 25 μ-thick discs (3600 discs total). The Discs have holes in the middle to let particles effuse through the target to a connection tube then to the ionizer. Figure 1 illustrates the target geometry and the effusion path of a single atom.

Earlier analysis of the release curves obtained with the RIST target at ISOLDE were presented in [8] and [9]. The present effort is to simulate this target with a detailed 3-D model using the Geant-4 tool kit described above. The simulation is performed for the experimental conditions at ISOLDE to study the release of ^{8}Li at a temperature of 1950 ^{o}C. The result of the simulation is compared to the data in order to identify the dominant process in the release and extract important parameters like diffusion coefficient and sticking time.

The result of the effusion part shows that particles collide about 2.5×10^{6} times with the target surface and travel 300 m on the average before exiting the ionizer. This corresponds to an average flight time of about 120 ms for ^{8}Li at 1950 ^{o}C. The sticking time and the diffusion coefficient (diffusion time) are free parameters to be determined by fit to the data.

The best fit of the simulated release curve to the experimental one was obtained for a sticking time per collision $\tau_s = 0\,ns$ (or $< 1\,ns$) and any value of the diffusion coefficient $D \leq 10^{-7}\,cm^2/s$, see figure 2-top. For example, using D of $10^{-8}\,cm^2/s$ gives exactly the same release curve as D of $10^{-7}\,cm^2/s$ after re-normalizing. This lack of sensitivity of the release curve to the value of D beyond an upper limit $D \sim 10^{-7}\,cm^2/s$ is due to the fact that the absolute normalization of the data is unknown. The lifetime of ^8Li is too short to determine D without supplemental information from a longer-lived isotope.

To better determine D, release data from stable isotopes measured over a longer time interval can be used. In a recent measurement by R. Bennett et al [10], a value of $D = 10^{-8}\,cm^2/s$ was obtained for ^7Li, the closest stable isotope to ^8Li. We will use this value for the rest of the paper.

In the bottom part of figure 2, we notice that the simulated release curve doesn't fit perfectly the shape of the experimental one, it is slightly faster. This could be explained by either a non uniform temperature in the target (existence of hot spots could result in a faster release) or an acceleration of ions in the electric field of the ion source. We will examine these two effects in the next section and see if we can reproduce the enhancement in the data.

4 Other effects : Temperature and Electric Field

4.1 Non uniform temperature in the target

The target temperature could be non uniform in space : some spots are hotter than others, or in time : extra heating during the beam pulse. This could make some particles exit much faster than others. To simulate this effect, we will consider two different diffusion components; one fast and one slow. In our case, the slow component is $D = 10^{-8}\, cm^2/s$ to which we will add a faster one. After trying different values, it appears that $D = 10^{-5}\, cm^2/s$ is the most appropriate value for the fast component.

The idea is to vary the contribution of the fast component in order to obtain a better fit to the experimental curve. Figure 3 shows that by increasing the contribution of the fast component, the simulated release curve is enhanced; the release is faster. A good fit is obtained for a contribution of about 0.9 %, see figure 3-bottom.

4.2 Electric field in the ionizer

The ionizer's heating current could induce an electric field which could accelerate ionized particles toward the exit and make the release faster. This effect acts as if the effective length of the ionizer were shorter, it can then be simulated by shortening the ionizer.

As shown in figure 4, making the ionizer shorter enhances the release. A very good fit is obtained with an ionizer's effective length of about 2 cm, almost the half of its physical length (3.5 cm). If this effect is real, then reversing the potential of the ionizer tube heater will dramatically change the release curve.

Although the fit obtained by varying the ionizer length is better than adding a fast component, we can't decide which effect is really acting, it could be both. We need dedicated measurements to know. For the rest of the paper, we will consider the ionizer to be responsible for the enhancement in the data, because it is easier to deal with only one diffusion coefficient.

Using $D = 10^{-8}\, cm^2/s$, $\tau_s = 0\, ns$ and an ionizer's effective length of 2 cm, the average effusion and diffusion times are 0.075 s and 52 s respectively. It is then clear that the diffusion is the dominant process in the release of ^8Li from the RIST target. The efficiency is estimated to be about 8% which is mainly due to the very long diffusion time $\tau_d = 63.3\, s$ compared to the ^8Li half life $T_{1/2} = 0.84\, s$.

In the next section we will discuss two possible ways to optimize the target geometry in order to improve the efficiency.

5 Optimizing the geometry

In order to make the release faster and increase the target efficiency, we have considered two effects. First the ionizer length which will affect only the effusion time. We have seen (figure 4) that shortening the ionizer enhances the release. Second the thickness of the discs, which is diffusion related and for which we expect a significant impact since the diffusion time τ_d is proportional to the square of the thickness d. Reducing the thickness by a factor 2 will reduce the diffusion time by a factor 4.

The question here is : to what extent this will affect the total delay time and the target efficiency ?

5.1 Shorter Ionizer

Making the ionizer shorter reduces the chance for a particle to go back inside the target volume which reduces the number of bounces and the total path length. Table 1 compares the result obtained for different ionizer lengths.

Shortening the ionizer from its original length ($3.5\,cm$) to about third length ($1\,cm$) reduces the average number of collision and path length by a factor of $\sim$ 2.5 and increases the target efficiency by 6% for ^{8}Li and 100% for ^{11}Li. The effect is amplified for ^{11}Li because of its very short half life : $8.7\,ms$. We can conclude that the ionizer length should be the shortest possible when dealing with very short lived isotopes like $^{11}Li\,(8.7\,ms)$.

5.2 Thinner discs

The simulation of the same target with $2.5\,\mu$ discs, one tenth of the original thickness, and the same parameters as before ($D = 10^{-8}\,cm^2/s$, $\tau_s \leq 1\,ns$ and $l = 2\,cm$) results in an efficiency of about 67% for ^{8}Li , eight times more than the original configuration, ten times for ^{11}Li, see Table-2.

Table 2 shows that reducing the disc thickness by a factor ten, will amplify the number of bounces by a factor ten, which could be critical for sticky particles. In this case, effusion could dominate and we won't gain much or could even lose by reducing the disc thickness. The mean path length didn't change because the empty space available for particles is the same in both geometries.

In the light of this study we may conclude that by determining the important parameters of the release process, it is possible to optimize the target geometry in order to improve its efficiency to produce higher intensity radioactive beams and beams of very rare isotopes. The optimal parameters are ion species dependent.

6 Conclusion and Future Plans

A general method for simulating release curves for ISOL targets has been developed. It is based on a standard analytical treatment of the diffusion of radioisotopes from the target material and a general Monte Carlo treatment of the effusion process from the target area to the ion source. Detailed 3-dimensional geometries for the effusion process are modeled by the C++ code Geant-4, and the ions are tracked via a new physics subroutine written for this code package. The limiting elements for the diffusion/effusion processes can be identified by this simulation model, leading to predictions for improvements in extraction times and overall efficiencies of the ISOL method.

The Monte Carlo calculations for the RIST target geometry are time consuming on present Linux-based PC systems. The present calculations for the $2.5\,\mu m$ foil case took up to a week running as background jobs on a cluster of 10 such PC's. To speed up the process of optimizing ISOL target designs, we have proceeded towards parallelizing our codes to run on multi-processor machines like NERSC's supercomputers. This has been done using the "Message Passing Interface" Library, MPI [11]. A test run has already been performed successfully on the PDSF Linux cluster of NERSC. This will permit simulations of more complicated targets such as those filled with fibers or grains.

Since experimental data are necessary to determine the sticking time, τ_s, and the diffusion coefficient, D, for a specific element, we are currently collaborating with Oak Ridge National Laboratory. First, to use their recent effusion measurements for rare gases [12] and, second, to perform other measurements in order to characterize the effusion and determine the sticking time of various gases and material combinations. Furthermore, diffusion measurements at the UNISOR/ORNL facility will complement the effusion studies and enable complete modeling of realistic ISOL targets.

References

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Table 1 : Ionizer length effect. Efficiencies for ^{11}Li are calculated using the same diffusion coefficient and sticking time as for ^{8}Li to show the effect of the nuclide's life time : $840\,ms$ for ^{8}Li and $8.7\,ms$ for ^{11}Li.

Ionizer length	$3.5\,cm$	$2\,cm$	$1\,cm$
$< N_{collisions} >$	2.4×10^6	1.6×10^6	1.0×10^6
$< Path\,length > (m)$	290	190	120
$< Effusion\,time > (s)$	0.115	0.075	0.048
$Efficiency\,for\,^{8}Li\,(\%)$	8.0	8.3	8.5
$Efficiency\,for\,^{11}Li\,(\%)$	0.07	0.10	0.15

Table 2 : Disc thickness effect. Effusion time is determined using a sticking time of 0ns at each collision. The efficiency for ^{11}Li is calculated using the same diffusion coefficient and sticking time as for ^{8}Li.

Disc thickness	$25\,\mu$	$2.5\,\mu$
$< N_{collisions} >$	1.6×10^6	1.6×10^7
$< Path\,length > (m)$	190	190
$< Diffusion\,time > (s)$	52.1	0.521
$Efficiency\,for\,^{8}Li\,(\%)$	8.3	67
$Efficiency\,for\,^{11}Li\,(\%)$	0.1	1.0

Figure captions :

Figure 1 : Geometry of the RIST target showing the path of one particle from production to release

Figure 2 : Top : effect of the diffusion coefficient on the release curve. Middle : effect of sticking time on the release curve. Bottom : best fit of ^{8}Li release curve by varying the diffusion coefficient D and the sticking time per collision τ_s , obtained for $D \leq 10^{-7}\, cm^2/s$ and $\tau_s = 0\, ns$. The fit is constrained by the tail which is determined by the decay.

Figure 3 : Top : Effect of a non uniform temperature in the target by varying the contribution of the fast diffusion component. Bottom : Best fit obtained by varying the contribution of the fast component (0.9 %).

Figure 4 : Top : Effect of the electric field in the ioniser by shortening the ionizer's effective length. Bottom : Best fit obtained by varying the effective length of the ionizer

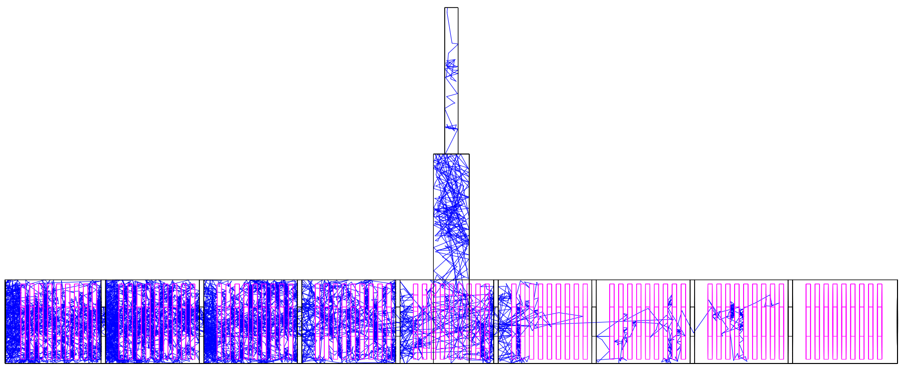

Figure 1.

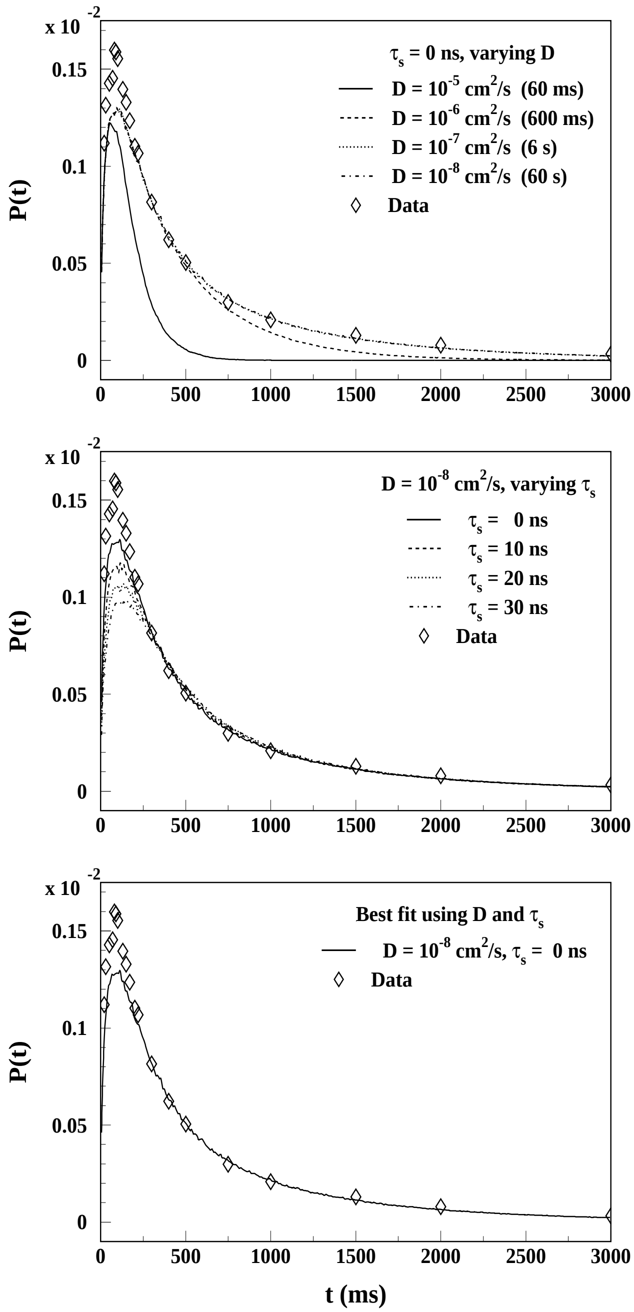
x 10^-2
τs = 0 ns, varying D
D = 10^-5 cm^2/s (60 ms)
D = 10^-6 cm^2/s (600 ms)
D = 10^-7 cm^2/s (6 s)
D = 10^-8 cm^2/s (60 s)
Data
P(t)
0.15
0.1
0.05
0
0
500
1000
1500
2000
2500
3000
D = 10^-8 cm^2/s, varying τs
τs = 0 ns
τs = 10 ns
τs = 20 ns
τs = 30 ns
Best fit using D and τs
D = 10^-8 cm^2/s, τs = 0 ns
t (ms)

Figure 2.

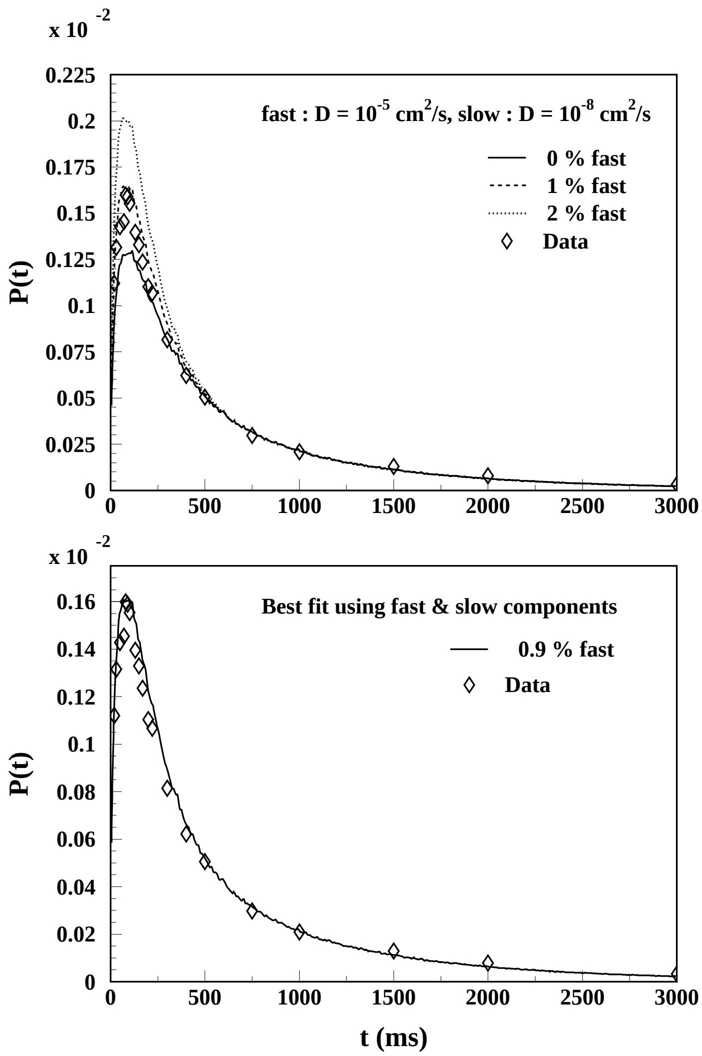
x 10 -2
0.225
0.2
0.175
0.15
0.125
0.1
0.075
0.05
0.025
0
P(t)
fast : D = 10-5 cm2/s, slow : D = 10-8 cm2/s
0 % fast
1 % fast
2 % fast
Data
0
500
1000
1500
2000
2500
3000
x 10 -2
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
P(t)
Best fit using fast & slow components
0.9 % fast
Data
t (ms)

Figure 3.

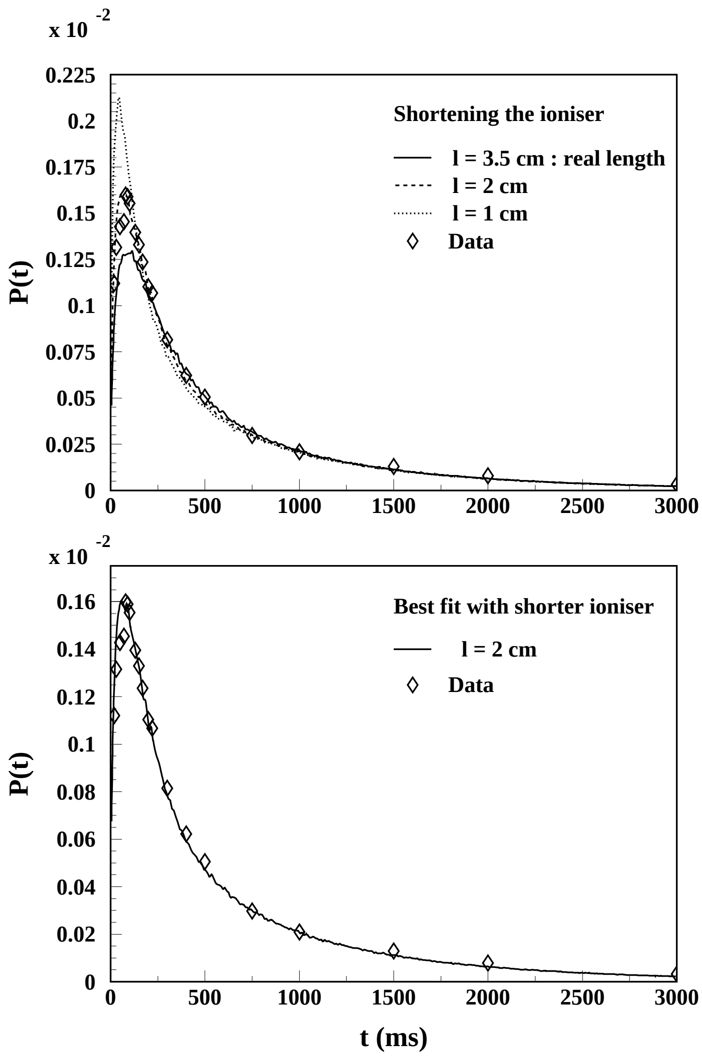
x 10 -2
Shortening the ioniser
l = 3.5 cm : real length
l = 2 cm
l = 1 cm
Data
P(t)
0.225
0.2
0.175
0.15
0.125
0.1
0.075
0.05
0.025
0
0
500
1000
1500
2000
2500
3000
x 10 -2
Best fit with shorter ioniser
l = 2 cm
Data
P(t)
0.16
0.14
0.12
0.1
0.08
0.06
0.04
0.02
0
t (ms)

Figure 4.